Dynamical linked cluster expansions: Algorithmic aspects and applications

H. Meyer-Ortmanns * [a]and T. Reisz† [b]

[a]Institute of Theoretical Physics, Bergische Universität Wuppertal,
Gauss-Str.20, D-42097 Wuppertal, Germany

[b]Institute of Theoretical Physics, University of Heidelberg,
Philosophenweg 16, D-69120 Heidelberg, Germany

Dynamical linked cluster expansions are linked cluster expansions with hopping parameter terms endowed with their own dynamics. They amount to a generalization of series expansions from 2-point to point-link-point interactions. We outline an associated multiple-line graph theory involving extended notions of connectivity and indicate an algorithmic implementation of graphs. Fields of applications are SU(N) gauge Higgs systems within variational estimates, spin glasses and partially annealed neural networks. We present results for the critical line in an SU(2) gauge Higgs model for the electroweak phase transition. The results agree well with corresponding high precision Monte Carlo results.

1. INTRODUCTION

Linked cluster expansions (LCEs) provide an analytic alternative to large scale Monte Carlo simulations. They are convergent series expansions of thermodynamic quantities. Originally developed in the infinite volume, they have recently been generalized to the finite volume [1] so that the expansion allows for a finite size scaling analysis. If the expansion is performed to a high order in the hopping parameter, even the critical region becomes available from the symmetric phase in spite of the ansatz that the expansion is performed about an ultralocal decoupled system [2].

2. DLCEs

For linked cluster expansions the action is typically split according to

$$S(\phi, v) = \sum_{x\in\Lambda} S^{\circ}(\phi_x) - \frac{1}{2}\sum_{x,y\in\Lambda} v_{x,y}\phi_x\phi_y. \qquad (1)$$

Here S° denotes the ultralocal part of the action depending on generic fields Φ associated with single sites x of a lattice Λ. The second term represents a pair interaction between fields at points $x, y \in \Lambda$. A frequent choice for v_{xy} is a coupling between nearest neighbours of Λ, v_{xy} is proportional to the so called hopping parameter κ.

For dynamical linked cluster expansions the action is split into 2 ultralocal parts $S^{\circ}(\Phi_x)$ and $S^1(U_l)$ with $S^{\circ}(\Phi_x)$ as above and $S^1(U_l)$ a single link action, depending on a field U_l associated with link $l = (x, y)$ of the lattice, and a point-link-point interaction, depending on the hopping parameter κ implicitly via v_{xy}. It reads

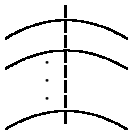
$$\begin{aligned} S(\phi, U, v) &= \sum_{x\in\Lambda} S^{\circ}(\phi_x) + \sum_{links\, l} S^1(U_l) \\ &\quad -\frac{1}{2}\sum_{x,y\in\Lambda} v_{xy}\phi_x U_{x,y}\phi_y. \end{aligned} \qquad (2)$$

Note that the former constant parameter v_{xy} gets replaced by $v_{xy}U_{xy}$ with U_{xy} obeying a dynamics governed by S^1. The action of (2) includes SU(N) gauge Higgs systems within variational estimates, spin glasses, partially annealed neural networks, but also generalizes to QCD with dynamical fermions if a suitable variational ansatz is made. From a systematic point of view, the generalization from 2-point interactions in a hopping term of an LCE to a point-link-point inter-

*e-mail: ortmanns@theorie.physik.uni-wuppertal.de
†e-mail: reisz@thphys.uni-heidelberg.de, supported by a Heisenberg fellowship

action in the hopping term of the class of actions in (2) amounts to a first step in the generalization to series expansions for n-point interactions with $n > 2$. The graphical expansion for DLCEs arises from a Taylor expansion of $\ln Z(H_x, I_l, v)$ about $v = 0$ with external sources H, I.

In DLCEs a new type of connectivity arises. While formerly vertices are connected via lines, here, in addition, lines are connected via a new type of vertices, represented by a dashed line, with



$$\Big\} \nu = \left(\frac{\partial^\nu W(I)}{\partial I_l^\nu}\right)_{I=v=0} \quad (3)$$

and $W = \ln Z$. Graphical expansions for correlation functions are generated from an expansion of W by attaching external Φ-lines and U-lines.

We remark that the usual LCE is included in a DLCE for frozen U-dynamics. Formally all multiple lines with $n > 1$ are absent because $\partial^n W(I)/\partial^n I_l = 0$ for $n > 1$.

Multiple-line (m-line) graph theory. A complete multiple-line graph theory has been formulated in [3]. Here we only summarize the most important notions out of a glossary which can be found in [3].

A multiple-line graph is a structure

$$\Gamma = (\mathcal{L}_\Gamma, \mathcal{M}_\Gamma, \mathcal{B}_\Gamma, E_\Gamma^{(\phi)}, E_\Gamma^{(U)}, \Phi_\Gamma, \Psi_\Gamma). \quad (4)$$

in which $\mathcal{L}_\Gamma$, $\mathcal{M}_\Gamma$, $\mathcal{B}_\Gamma$ are three mutually disjoint sets of bare internal lines, multiple-lines, and vertices of Γ, respectively. $E_\Gamma^{(\Phi)}$ and $E_\Gamma^{(U)}$ are maps that assign to every vertex v, multiple-line m the number of external Φ-lines, external U-lines to v, m, respectively. Finally, Φ_Γ and Ψ_Γ are incidence relations that assign bare internal lines to their endpoint vertices and to their multiple-lines, respectively.

The central notion of *multiple-line connectivity* can be traced back to the familiar notion of connectivity of LCE graphs by introducing auxiliary graphs. *Topological equivalence* of multiple line graphs is formulated by means of incidence relations. Certain operations on graphs must be defined such as the removal, the decomposition of an m-line or the decomposition of a vertex. To characterize equivalence classes of graphs, we define notions like **1LI** (1-line irreducible), **1VI** (1-vertex irreducible), and **1MLI** (1-multiple-line irreducible). The definitions as well as further details can be found in [3].

Algorithmic aspects. An algorithmic construction of the graphs which contribute to the n-point susceptibilities is the first step for a fully automatized computer implementation of the generation of graphs. In the following we specify a possible set of modules in the generation of DLCE-graph classes. We start with the class

$\mathcal{P}_1(L)$: the set of connected 1LI LCE vacuum graphs with l internal lines. Apart from certain exceptions this set contains graphs whose vertices are connected by just one line. For the precise definition we refer to [2]. The next module is

$\mathcal{P}_2(L)$: the set of connected 1LI LCE vacuum graphs with L internal lines whose vertices may be connected by any number of bare lines. In the usual LCE one would attach external lines in the next steps. In a DLCE we have first to generalize the set of LCE vacuum graphs to include graphs with dashed lines and resolved vertices. This way we are led to the classes

$\widetilde{\mathcal{MP}}_2(L)$: the set of 1LI m-line vacuum graphs with L internal bare lines so that all bare lines of an m-line have the same endpoint vertices and

$\mathcal{MP}_2(L)$: the set of all 1LI m-line vacuum graphs with L internal lines. In particular this class contains graphs that would be disconnected without dashed lines. In the next modules we attach external Φ-lines and U-lines in specific ways and obtain

$\mathcal{Q}_k(L)$: the set of renormalized vertex moment graphs with k external Φ-lines and L internal lines that are 1LI and have just one external vertex and no external m-line.

$\mathcal{R}_k(L)$: the set of renormalized m-line moment graphs with k external U-lines and L internal lines that are 1LI and have just one external m-line, but no external vertex.

$\mathcal{S}_{E_1,E_2}(L)$: the set of graphs with E_1 external Φ-lines, E_2 external U-lines and L internal lines that are both 1VI and 1MLI. Because of certain factorization properties of the corresponding analytic expressions, graphs of $\mathcal{Q}_k(L)$ $\mathcal{R}_k(L)$, and $\mathcal{S}_{E_1,E_2}(L)$ can be patched together to yield the

full set of connected 1LI DLCE graphs.

The additional type of connectivity leads to a pronounced proliferation of DLCE graphs as compared to the LCE graphs for the same order in the number of internal lines. As an example let us consider the 2-point susceptibility χ_2. The ratio of the number of DLCE to LCE graphs contributing to χ_2 to $O(\kappa^4)$ is already 80/8. Once the algorithmic generation of DLCE graphs is implemented on a computer, the critical region of a variety of systems will become available in spite of the ponounced proliferation of graphs.

3. Applications

The SU(2) Higgs model. The action of the SU(2) Higgs model in 4 dimensions does not quite have the form to allow for a DLCE, because the Wilson part of the action is neither ultralocal nor of the type point-link-point. Therefore we have replaced the action by a variational ansatz that leads to a factorization of the partition function over time slices, whereas the action for the degrees of freedom along the 3-d spacelike hypersurfaces takes a form that is included as a special case of Eq. (2). The precise form can be found in [3]. The equations that determine the optimal choice of variational parameters are solved by means of a DLCE in 3 dimensions. Here we directly state one particular result for the critical line of the electroweak transition in the SU(2) Higgs model. It refers to κ_{crit} at $\lambda = 5.0 \cdot 10^{-4}$ and $\beta = 8.0$.

Method	lattice	κ_{crit}
Monte Carlo	$2 \cdot 32 \cdot 32 \cdot 256$	0.12887(1)
DLCE	$4 \cdot \infty^3$	0.1282(1)

The Monte Carlo data are taken from Fodor et al. [4]. "DLCE" refers to variational estimates in combination with DLCEs in which expectation values are evaluated including terms of $O(\kappa^4)$. Such a moderate order in the expansion may hide the complexity of the analysis [5]. The total number of graphs contributing to the variational equations is about several hundred. Thus the good quantitative agreement with the high precision Monte Carlo results of Fodor et al. is not so surprising. In addition we have been lucky in the choice of variational ansatz. The 3-dimensional spacelike hypersurfaces are expected to contain the nonperturbative degrees of freedom that drive the Higgs transition, whereas the mean field treatment of the timelike degrees of freedom seems to be a reasonable approximation, although the temperature dependence gets lost this way by construction.

Avoiding the replica trick in spin glasses. The quantity that is of actual interest in spin glasses is $[[lnZ_\beta(U)]]$ in which Z_β denotes the partition function of a spin system at inverse temperature β for given interactions (couplings) U. $[[\cdots]]$ denotes an average over U w.r.t. a probability distribution governed by an action of the type of S^1, cf. (2). Usually the replica trick involves an uncontrolled extrapolation from integer to real numbers. In contrast to that we have shown in [3] that $[[\ln Z_\beta(U)]]$ can be directly evaluated in a modified type of DLCE. As a series representation we have

$$[[\frac{1}{V} \ln Z_\beta(U)]] \ = \ \sum_{L \geq 0} (2K)^L \sum_{\Delta} w(\Delta). \qquad (5)$$

The sum runs over all graphs Δ that belong to $\widetilde{\mathcal{G}}_{0,0}(L)$, the subset of multiple-line vacuum graphs with L internal lines that stay connected without any dashed lines in the usual LCE sense. In (5) $w(\Delta)$ denotes the full analytic weight of the graph Δ, its explicit expression can be found in [3].

We expect that the DLCE series in (5) is convergent for a large class of interactions for which the set $\widetilde{\mathcal{G}_{0,0}}(L)$ can be further restricted to certain subclasses.

REFERENCES

1. H. Meyer-Ortmanns and T. Reisz, J. Stat. Phys. 87 (1997) 755.
2. T. Reisz, Phys. Lett. B360 (1995) 77; T. Reisz, Nucl. Phys. B450 (1995) 569.
3. H. Meyer-Ortmanns and T. Reisz, Int. J. Mod. Phys. A (1998), in press.
4. Z. Fodor et al., Nucl. Phys. B439 (1995) 147.
5. H. Meyer-Ortmanns and T. Reisz, in preparation.